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GENERALIZATION OF LAPLACE'S EXPANSION TO ARBITRARY
POWERS AND FUNCTIONS OF THE DISTANCE
BETWEEN TWO POINTS

by

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Addenda and Errata to WIS-TCI-20 - "Generalization of Laplace's Expansion to Arbitrary Powers and Functions of the Distance Between Two Points"

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Abstract Last line, replace "$f\,(r_1^2 + r_2^2)^{\frac{1}{2}}$" by "$f\left[(r_1^2 + r_2^2)^{\frac{1}{2}}\right]$".

Page 1 Footnote 1, "Sitgungsberichte" should read "Sitzungsberichte".

Page 3 Line 17, replace "as well as of" by "as well as on".

Page 3 Last line, should read "$G_{n\ell}(x)$ is an ..."

Page 4 Last line, "of the degree" should read "in n of a degree".

Page 6 Two lines below Eq. 23, replace "$n < -2$" with "$n \leq -2$".

Page 6 Nine lines below Eq. 23, replace "$(r_>^2 - r_<^2)/r^2$" with "$(r_>^2 - r_<^2)/r_>^2$".

Page 7 Eq. 26b, "$(1+\gamma x)^{-2}$" should read "$(1+\gamma x)^{-2\alpha}$".

Page 8 Line 1, replace "$(-\frac{1}{2}n)^{\ell}$" with "$(-\frac{1}{2}n)_{\ell}$".

Page 8 Four lines below Eq. 28, "(25a)" should read "(27a)".

Page 14 Eq. 55, replace "$f \; =$" with "$f_{\ell} =$".

Page 15 Three lines below Eq. 59, replace "$(\pi/2r)^{\frac{1}{2}}$" with "$(\pi/2z)^{\frac{1}{2}}$".

Page 16 Two lines below Eq. 63b, replace $\ell = \frac{1}{2}$ with $\nu = \frac{1}{2}$.

Eq. (57) on page 14 should read:

$$j_o(kr) = \sin(kr)/(kr) \quad , \quad y_o(kr) = -\cos(kr)/(kr)$$

$$h_o^{(1)}(kr) = -ie^{ikr}/(kr) \quad , \quad h_o^{(2)}(kr) = ie^{-ikr}/(kr) \qquad (57)$$

GENERALIZATION OF LAPLACE'S EXPANSION TO ARBITRARY POWERS AND FUNCTIONS OF THE DISTANCE BETWEEN TWO POINTS*

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ABSTRACT

In analogy to Laplace's expansion, an arbitrary power r^n of the distance r between two points, $(r_1, \vartheta_1, \varphi_1)$ and $(r_2, \vartheta_2, \varphi_2)$, is expanded in terms of Legendre polynomials of $\cos \vartheta_{12}$. The coefficients are homogeneous functions of r_1 and r_2 of degree n satisfying simple differential equations; they are solved in terms of Gauss' hypergeometric functions of the variable $(r_< / r_>)$. The transformation theory of hypergeometric functions is applied to describe the nature of the singularities as r_1 tends to r_2 and of the analytic continuation of the functions past these singularities. Expressions symmetric in r_1 and r_2 are obtained by quadratic transformations; for $n = -1$, one of these has previously been given by Fontana. Some 3-term recurrence relations between the radial functions are established, and the expressions for the logarithm and the inverse square of the distance are discussed in detail.

For arbitrary analytic functions $f(r)$ three analogous expansions are derived; the radial dependence involves spherical Bessel functions of $(r_< \partial/\partial r_>)$ or of related operators acting on $f(r_>)$, $f(r_1 + r_2)$ or $f\ (r_1^{\,2} + r_2^{\,2})^{\frac{1}{2}}$.

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GENERALIZATION OF LAPLACE'S EXPANSION TO ARBITRARY POWERS AND FUNCTIONS OF THE DISTANCE BETWEEN TWO POINTS

1. Introduction

The inverse distance r^{-1} between two points Q_1 and Q_2 specified by the polar coordinates $(r_1, \vartheta_1, \varphi_1)$ and $(r_2, \vartheta_2, \varphi_2)$ with reference to a common origin O is given by the well-known Laplace expansion

$$r^{-1} = r_>^{-1} \sum_{\ell=0}^{\infty} (r_< / r_>)^{\ell} \; P_{\ell} \; (\cos \vartheta_{12}) \tag{1}$$

where

$$r_< = \min (r_1, r_2) \; , \; r_> = \max (r_1, r_2) \quad , \tag{2}$$

$$\cos \vartheta_{12} = \cos \vartheta_1 \cos \vartheta_2 + \sin \vartheta_1 \sin \vartheta_2 \cos(\varphi_1 - \varphi_2) \tag{3}$$

and the $P_{\ell}(x)$ are the Legendre polynomials. In many physical problems, the distance between Q_1 and Q_2 may be required to powers other than the inverse first, and an expansion analogous to (1) is required for such cases. One way of approaching the problem is to preserve the expansion in powers of $(r_< / r_>)$; the expression

$$r^{-2N} = r_>^{-2N} \sum_{\ell=0}^{\infty} (r_< / r_>)^{\ell} \; C_{\ell}^{N} (\cos \vartheta_{12}) \tag{4}$$

serves to define the angular dependence as Gegenbauer polynomials of the argument[1] (cf. B 3.15[2]); but for three-dimensional problems it is more convenient to preserve the dependence on the angles, and to

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[1] L. Gegenbauer, Wiener Sitgungsberichte, 70, 6, 434 (1874); 75, 891 (1877).

[2] Bateman Manuscript Project, A. Erdélyi (Ed.), Higher Transcendental Functions, (McGraw-Hill Book Company, Inc., New York, 1953). Sections and formulas in this work will be directly referenced by the letter B .

re-define the dependence on the radii, and the writer is not aware that the corresponding expansion

$$V_n = r^n = \sum_{\ell} R_{n\ell}(r_1, r_2) P_\ell(\cos\vartheta_{12}) \qquad (5)$$

has been given in the general case. If n is a positive even integer, V_n is the $(\frac{1}{2}n)$th power of

$$r^2 = r_1^2 + r_2^2 - 2r_1 r_2 \cos\vartheta_{12} \qquad (6)$$

and the expansion (5) will be a finite series terminating with $\ell = \frac{1}{2}n$; the form of the radial functions R_n is independent of the comparative values of r_1 and r_2. For odd positive values of n recurrence relations based on (1) and (6) have occasionally been quoted; the expressions for $n = 1$ have been given explicitly by Jen[3].

The purpose of the present paper is to derive the explicit terms in the expansion (5) for the general case. For variations of the positions of the points Q_1 and Q_2 the function V_n appears as the solution of the partial differential equation

$$\nabla_1^2 V_n = \nabla_2^2 V_n = n(n+1) V_{n-2} \quad ; \qquad (7)$$

the corresponding differential equation for the radial functions R_n following from (5) and (7), together with simple additional conditions of dimensionality and continuity, are solved in section 2 in terms of Gauss' hypergeometric function

$$F(\alpha, \beta; \gamma, x) = 1 + \sum_1^\infty \frac{(\alpha)_s (\beta)_s}{(\gamma)_s \, s!} x^s \qquad (8)$$

where

$$(\alpha)_0 = 1 \; ; \quad (\alpha)_s = \alpha(\alpha+1)\cdots(\alpha+s-1) = \Gamma(\alpha+s)/\Gamma(\alpha) \quad . \qquad (9)$$

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[3] C. K. Jen, Phys. Rev., 43, 540 (1933).

In section 3 the extensive transformation theory of the hypergeometric function is applied to express the R_n in a variety of forms and to study their behaviour, especially in the asymptotic case $r_1 \to r_2$. The results obtained are asymmetric in $r_<$ and $r_>$, but by means of quadratic transformations can be expressed in several symmetric forms; for $n = -1$ one of these transformations has recently been derived by Fontana[4] on the basis of group-theoretical arguments.

In section 4 Gauss' relations between contiguous hypergeometric functions are used to establish recurrence relations between the R_n, and the case of the logarithm and the inverse square are discussed in greater detail in section 5.

The results obtained in section 3 are re-written in section 6 in a symbolic form, independent of the power n, but involving powers or functions of differential operators; this yields an expansion theorem for an arbitrary analytic function $f(r)$. The more general problem that the function depends on the relative orientation of Q_1 and Q_2 as well as of their distance will be considered in a separate paper.

2. Mathematical Derivation

Substitution of (7) into (5) leads to

$$\frac{\partial^2 R_{n\ell}}{\partial r_1^{\,2}} + \frac{2}{r_1}\frac{\partial R_{n\ell}}{\partial r_1} - \ell(\ell+1)\frac{R_{n\ell}}{r_1^{\,2}} = \frac{\partial^2 R_{n\ell}}{\partial r_2^{\,2}} + \frac{2}{r}\frac{\partial R_{n\ell}}{\partial r_2} - \ell(\ell+1)\frac{R_{n\ell}}{r_2^{\,2}} . \quad (10)$$

Furthermore the R_n are homogeneous functions of degree n in the variables r_1 and r_2, and since V_n is a continuous function if $r_< = 0$, they must contain the factor $r_<^{\ell}$ so that

$$R_{n\ell}(r_1,r_2) = r_<^{\ell} r_>^{n-\ell} G_{n\ell}(r_< / r_>) \quad (11)$$

where $G_{n,1}(x)$ is a analytic function for $0 \leq x < 1$.

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[4] P. R. Fontana, J. Mathematical Physics, 2, 825 (1961).

Expressing G_n as a power series

$$G_{n\ell}(r_< / r_>) = \sum_s c_{n\ell s}(r_< / r_>)^s \tag{12}$$

and substituting (10) into (11) we obtain the recurrence relations

$$(s+2)(2\ell+s+3)c_{n,\ell,s+2} = (n-2\ell-s)(n-s-1)c_{n\ell s} \quad . \tag{13}$$

The sequence of coefficients thus begins with $s = 0$ as the other possibility $s = -2\ell-1$ would violate the continuity condition, and hence $c_{n\ell s} = 0$ for odd s, and for even $s = 2\nu$

$$c_{n,\ell,2\nu} = \frac{(\ell-\frac{1}{2}n)_\nu \; (-\frac{1}{2}n-\frac{1}{2})_\nu}{(\ell+3/2)_\nu \; \nu!} c_{n\ell o} \tag{14}$$

where $(a)_\nu$ is defined in (9). Hence with the definition (8) for Gauss' hypergeometric function (11), (12) and (14) yield

$$R_{n\ell}(r_1, r_2) = K(n,\ell)\, r_<^{\ell} r_>^{n-\ell} F\left(\ell-\tfrac{1}{2}n, -\tfrac{1}{2}-\tfrac{1}{2}n;\ \ell+\tfrac{3}{2};\ \frac{r_<^2}{r_>^2}\right) \quad . \tag{15}$$

The coefficients $K(n,\ell)$ are most easily determined by considering the case $\vartheta_{12} = 0$ when all the $P_\ell(\cos\vartheta_{12}) = 1$:

$$V_n = |r_> - r_<|^n = r_>^n \sum_\lambda \binom{n}{\lambda} \left(\frac{-r_<}{r_>}\right)^\lambda \quad ; \tag{16}$$

comparison of the coefficients of $r_<^\lambda r_>^{n-\lambda}$ in (15) and (16) yields

$$\begin{aligned}\frac{n(n-1)\cdots(n-\lambda+1)}{\lambda!} = {} & K(n,\lambda) + K(n,\lambda-2)\,\frac{(\lambda-2-\frac{1}{2}n)(-\frac{1}{2}-\frac{1}{2}n)}{\lambda-\frac{1}{2}} \\ & + K(n,\lambda-4)\,\frac{(\lambda-4-\frac{1}{2}n)_2\,(-\frac{1}{2}-\frac{1}{2}n)_2}{(\lambda-\frac{5}{2})_2\;2!} + \cdots \quad .\end{aligned} \tag{17}$$

Considered as a function of n the left hand side is polynomial of degree λ; it follows by induction that each $K(n,\ell)$ must be a polynomial of the degree not exceeding ℓ.

Now for positive even ℓ the series (17) breaks off at $\ell = \frac{1}{2}n$, and conversely for any value of ℓ $K(n,\ell)$ vanishes for $n = 0, 2, \cdots 2\ell - 2$. Hence it must be a multiple of $n(n-2)\cdots(n-2\ell+2)$ or of $(-\frac{1}{2}n)_\ell$ and since by virtue of (1) all $K(-1,\ell)$ are unity, the general solution is

$$K(n,\ell) = (-\tfrac{1}{2}n)_\ell / (\tfrac{1}{2})_\ell \quad . \tag{18}$$

3. Solution for the Radial Functions and their Transformations

The equations (15) and (18) show that radial functions $R(n,\ell)$ in the expansion (5) are given as

$$R_n(r_1,r_2) = \frac{(-\frac{1}{2}n)_\ell}{(\frac{1}{2})_\ell} r_>^{\,n} \left(\frac{r_<}{r_>}\right)^\ell F\left(\ell - \tfrac{1}{2}n, -\tfrac{1}{2}-\tfrac{1}{2}n; \ell + \tfrac{3}{2}; \frac{r_<^2}{r_>^2}\right) \quad . \tag{19}$$

The hypergeometric functions (8) are finite series, i.e. they are polynomials in x, if either α or β is a negative integer or zero. This implies that for all positive odd integer values the series for $R_{n\ell}$ break off, and if $n = -1$ they consist of the leading term only, in agreement with (1). For positive even n the series are finite for $\ell \leq \frac{1}{2}n$; for $\ell > \frac{1}{2}n$ the factor $(-\frac{1}{2}n)_\ell$ ensures that R_n vanishes identically.

Of the numerous transformations of the hypergeometric function the following are expecially relevant in the present context (cf. B 2.9.1,2; B 2.10.1,2):

$$F(\alpha,\beta;\gamma;x) = (1-x)^{\gamma-\alpha-\beta} F(\gamma-\alpha,\gamma-\beta;\gamma;x) \tag{20a}$$

$$= \frac{\Gamma(\gamma)\Gamma(\gamma-\alpha-\beta)}{\Gamma(\gamma-\alpha)\Gamma(\gamma-\beta)} F(\alpha,\beta;\alpha+\beta-\gamma+1;1-x) + \\ + \frac{\Gamma(\gamma)\Gamma(\alpha+\beta-\gamma)}{\Gamma(\alpha)\Gamma(\beta)} (1-x)^{\gamma-\alpha-\beta} F(\gamma-\alpha,\gamma-\beta;\gamma-\alpha-\beta+1;1-x) \tag{20b}$$

$$= \frac{\Gamma(\gamma)\Gamma(\beta-\alpha)}{\Gamma(\beta)\Gamma(\gamma-\alpha)} (-x)^{-\alpha} F(\alpha,1-\gamma+\alpha;1-\beta+\alpha;x^{-1}) + \\ + \frac{\Gamma(\gamma)\Gamma(\alpha-\beta)}{\Gamma(\alpha)\Gamma(\gamma-\beta)} (-x)^{-\beta} F(\beta,1-\gamma+\beta;1-\alpha+\beta;x^{-1}) \tag{20c}$$

The first, if applied to (19), yields

$$R_{n\ell}(r_1,r_2) = \frac{(-\frac{1}{2}n)_\ell}{(\frac{1}{2})_\ell} \frac{r_<^\ell (r_>^2-r_<^2)^{n+2}}{r_>^{\ell+n+4}} F\left[\ell+2+\tfrac{1}{2}n, \tfrac{3}{2}+\tfrac{1}{2}n; \ell+\tfrac{3}{2}; \frac{r_<^2}{r_>^2}\right], \tag{21}$$

which shows that the functions F are invariant against the substitution $n \to -n-4$. Thus the coefficients R are rational functions of r_1 and r_2 for odd integer n whatever its sign, and also for negative even n as long as $\ell < \frac{1}{2}|n|-1$, though in the latter case the expansion (5) does not break off as with positive even n.

The transformation (20b) applied to (19) yields

$$R_{n\ell}(r_1,r_2) = \frac{2^{n+1}(\ell+\frac{1}{2})(-\frac{1}{2}n)_\ell}{(1+\frac{1}{2}n)_{\ell+1}} r_<^\ell r_>^{n-\ell} F\left[\ell-\tfrac{1}{2}n, -\tfrac{1}{2}-\tfrac{1}{2}n; -1-n; \frac{r_>^2-r_<^2}{r_>^2}\right]$$

$$- \frac{2\ell+1}{2^{n+3}(n+2)} \frac{r_<^\ell (r_>^2-r_<^2)^{n+2}}{r_>^{\ell+n+4}} F\left[\ell+\tfrac{1}{2}n+2, \tfrac{3}{2}+\tfrac{1}{2}n; n+3, \frac{r_>^2-r_<^2}{r_>^2}\right]. \tag{22}$$

Here the gamma-products have been simplified with the use of (9) and Legendre's duplication formula (B 1.3.15)

$$\Gamma(2z) = 2^{2z-1}\pi^{-\frac{1}{2}}\,\Gamma(z)\,\Gamma(z+\tfrac{1}{2}) . \tag{23}$$

The expansion (22) shows the nature of the branch point for fractional n as $r_<$ approaches $r_>$; we see that for $n < -2$ the individual functions R_n are divergent, though they remain integrable as long as $n > -3$.

For integer n (22) needs special interpretation as either one series contains terms with the indeterminate factor $0/0$, or else both series possess infinite coefficients. In particular, if the function F in (19) represents a polynomial in $r_<^2/r_>^2$, it transforms into a polynomial in the variable $(r_>^2-r_<^2)/r^2$; this corresponds to the terminating part of that series in (22) which has negative parameters; the terms of this series resume when the denominator in (8) also vanishes, a passage to the limit shows that the ratio $0/0$ is to be interpreted as $\frac{1}{2}$, and the resumed terms will exactly cancel the other series (22). On the other hand, for the non-terminating series R_n

in (19) at negative even n the infinities of the two series will cancel out, leading to logarithmic terms in agreement with (B 2.10.12,13).

The transformation (20c) when applied to (19) leads to

$$R_{n\ell} = \frac{(-\frac{1}{2}n)_\ell}{(\frac{1}{2})_\ell} (-1)^{\frac{1}{2}n} \cos\tfrac{1}{2}n\pi \; r_<^{n-\ell} r_>^{\ell} \; F\left(\ell-\tfrac{1}{2}n; -\tfrac{1}{2}-\tfrac{1}{2}n; \tfrac{3}{2}+\ell; \frac{r_>^2}{r_<^2}\right)$$

$$+ \frac{\Gamma(\ell+\frac{3}{2})\pi^{\frac{1}{2}}}{\Gamma(-\frac{1}{2}n)\,\Gamma(2+\ell+\frac{1}{2}n)} (-1)^{\frac{1}{2}(n+1)} r_<^{n+\ell+1} r_>^{-1-\ell} F\left(-1-\ell-\tfrac{1}{2}n, -\tfrac{1}{2}-\tfrac{1}{2}n; \tfrac{1}{2}-\ell; \frac{r_>^2}{r_<^2}\right), \tag{24}$$

the constant factor of the first series having been simplified by means of the relation (B 1.2.6)

$$\Gamma(z)\,\Gamma(1-z) = \pi/\sin\pi z \quad . \tag{25}$$

Equation (24) shows the nature of the analytic continuation of $R_{n\ell}$ from $r_1 < r_2$ to $r_1 > r_2$, or conversely. As expected, this agrees with the true expression (19) for $r_1 > r_2$ only if n is a non-negative even integer; in this case the second series in (23) has zero coefficient. For the non-terminating series $R_{n\ell}$ in the case of negative even n, the second term in (23) has a purely imaginary coefficient of indeterminate sign; the true function (19) for $r_1 > r_2$ corresponds to the first term in (23) only and is therefore not the analytic continuation of $R_{n\ell}$ for $r_1 < r_2$, but its Cauchy principal value with respect to the logarithmic singularity at $r_1 = r_2$.

The relations between the three parameters occurring in the hypergeometric function in (19) allow additional, quadratic transformations to be applied to the $R_{n\ell}$. Thus application of (B 2.11.34,36)

$$F(\alpha,\beta;\alpha-\beta+1;x) = (1+x)^{-\alpha} F\left[\tfrac{1}{2}\alpha, \tfrac{1}{2}\alpha+\tfrac{1}{2}; \alpha-\beta+1; 4x(1+x)^{-2}\right] \tag{26a}$$

$$= (1+\sqrt{x})^{-2} F\left[\alpha, \alpha-\beta+\tfrac{1}{2}; 2\alpha-2\beta+1; 4\sqrt{x}(1+\sqrt{x})^{-2}\right] \tag{26b}$$

to (19) leads to

$$R_{n\ell}(r_1,r_2) = \frac{(-\frac{1}{2}n)^{\ell}}{(\frac{1}{2})_{\ell}} \frac{(r_1r_2)^{\ell}}{(r_1^{\,2}+r_2^{\,2})^{\ell-\frac{1}{2}n}} F\left[\frac{\ell}{2}-\frac{n}{4}, \frac{\ell}{2}-\frac{n}{4}+\tfrac{1}{2}; \frac{3}{2}+\ell; \frac{4r_1^{\,2}r_2^{\,2}}{(r_1^{\,2}+r_2^{\,2})^2}\right] \tag{27a}$$

$$= \frac{(-\frac{1}{2}n)_{\ell}}{(\frac{1}{2})_{\ell}} \frac{(r_1r_2)^{\ell}}{(r_1+r_2)^{2\ell-n}} F\left[\ell-\tfrac{1}{2}n, 1+\ell; 2+2\ell; \frac{4r_1r_2}{(r_1+r_2)^2}\right] . \tag{27b}$$

These expressions are completely symmetric in r_1 and r_2, the asymmetry in (19) in the two variables is related to the transformations inverse to (26) and (27), (cf. B 2.11.6,31) which involve square roots which must be taken with a fixed sign. This leads to variables of the form

$$\frac{r_1^{\,2}+r_2^{\,2}-|r_1^{\,2}-r_2^{\,2}|}{r_1^{\,2}+r_2^{\,2}+|r_1^{\,2}-r_2^{\,2}|} \qquad \text{and} \qquad \left[\frac{r_1+r_2-|r_1-r_2|}{r_1+r_2+|r_1-r_2|}\right]^2 \tag{28}$$

both of which equal $r_<^{\,2}/r_>^{\,2}$ of (2). Similar considerations apply to the factor outside the hypergeometric function. Fontana[4] has derived by group theoretical methods an expression for $R_{-1,\ell}$ in terms of double factorials equivalent to (25a); a number of numerical results given in Fontana's paper thus appear as special cases of (26). For positive even n the functions F in (27) reduce to polynomials; but for odd n they are infinite series, so that the main advantage of (19) and (21) is lost by this transformation.

Hypergeometric functions which admit of quadratic transformations such as (26) are related to Legendre functions. Comparison of (27a) with (B 3.2.41) shows that the $R_n(r_1,r_2)$ can be expressed in terms of associated Legendre functions of the second kind $Q_{\ell}^{\mu}\left[(r_1^{\,2}+r_2^{\,2})/(2r_1r_2)\right]$, where $\mu = -1-\frac{1}{2}n$. Since however, the various definitions of Q_{ℓ}^{μ} for fractional μ involve differing phase angles, this approach will not be studied further.

4. Recurrence Relations

Any three contiguous hypergeometric functions, i.e. whose parameters differ by an integer only, satisfy a linear recurrence relation; hence there exists a linear relation between any three radial functions $R_{n\ell}(r_1,r_2)$, provided the values of ℓ differ by integers and those of n , by even integers. Thus application of (B 2.8.31) to (27b) yields

$$(4+2\ell+n)(2\ell-2-n)R_{n+2,\ell} + 2(2+n)^2(r_1^{\,2}+r_2^{\,2})R_{n\ell} - n(n+2)(r_1^{\,2}-r_2^{\,2})^2R_{n-2,\ell} = 0 \,, \tag{29}$$

of (B 2.9.3) and (B 2.8.45) to (19)

$$\frac{r_1^{\,2}+r_2^{\,2}}{r_1r_2}R_{n\ell} - \frac{\ell+2+\frac{1}{2}n}{\ell+\frac{3}{2}}R_{n,\ell+1} - \frac{\ell-1-\frac{1}{2}n}{\ell-\frac{1}{2}}R_{n,\ell-1} = 0 \quad , \tag{30}$$

and of (B 2.9.35) to (27a)

$$(r_1^{\,2}+r_2^{\,2})R_{n\ell} - \frac{2\ell+1}{\ell-\frac{1}{2}}r_1r_2R_{n,\ell-1} - \frac{2+\ell+\frac{1}{2}n}{1+\frac{1}{2}n}R_{n+2,\ell} \quad . \tag{31a}$$

Elimination of $R_{n,\ell-1}$ or $R_{n\ell}$ from (30) and (31a) leads to

$$(r_1^{\,2}+r_2^{\,2})R_{n\ell} - \frac{2\ell+1}{\ell+\frac{3}{2}}r_1r_2R_{n,\ell+1} + \frac{\ell-1-\frac{1}{2}n}{1+\frac{1}{2}n}R_{n+2,\ell} = 0 \tag{31b}$$

and

$$r_1r_2\left[\frac{R_{n,\ell+1}}{\ell+\frac{3}{2}} - \frac{R_{n,\ell-1}}{\ell-\frac{1}{2}}\right] - \frac{R_{n+2,\ell}}{1+\frac{1}{2}n} = 0 \tag{31c}$$

respectively, and application of (29) to (31a) and (31b) yields

$$n(r_1^{\,2}-r_2^{\,2})^2R_{n-2,\ell} = (2\ell+2+n)(r_1^{\,2}+r_2^{\,2})R_{n\ell} - (2\ell+1)(2\ell-2-n)r_1r_2R_{n,\ell-1}/(\ell-\tfrac{1}{2}) \tag{32a}$$

$$= -(2\ell-n)(r_1^{\,2}+r_2^{\,2})R_{n\ell} + (2\ell+1)(4+2\ell+n)r_1r_2R_{n,\ell+1}/(\ell+\tfrac{3}{2}) \;; \tag{32b}$$

with a renewed application of (30) this leads to

$$\frac{n(r_1^2-r_2^2)^2 R_{n-2,\ell}}{r_1 r_2} = 2\frac{(\ell+1+\frac{1}{2}n)_2}{\ell+\frac{3}{2}} R_{n,\ell+1} - 2\frac{(\ell-1-\frac{1}{2}n)_2}{\ell-\frac{1}{2}} R_{n,\ell-1} \quad . \tag{32c}$$

All these formulas are 3-term recurrence relations, independent of the relative magnitudes of r_1 and r_2 . As mentioned in the introduction use has previously been made of (6) to express $R_{n+2,\ell}$ in terms of $R_{n\ell}, R_{n,\ell-1}$ and $R_{n,\ell+1}$; such formulas are, of necessity, 4-term recurrence relations.

5. Explicit Formulas for the Logarithm and the Inverse Square

The expansion for $\log r$ corresponding to (5)

$$\log r = \sum R_{\log,\ell}(r_1,r_2) P_\ell(\cos\vartheta_{12}) \tag{34}$$

is most easily deduced from the limiting process

$$\log r = \lim \partial(r^n)/\partial n \qquad \text{as} \quad n \to 0 \quad . \tag{35}$$

The factor $(-\frac{1}{2}n)_\ell$, which occurs in the expressions for $R_{n\ell}$, vanishes for $n = 0$, $\ell > 0$, but gives a non-zero derivative; hence for all $\ell > 0$ we obtain from (19), (21) and (27)

$$R_{\log,\ell} = -\frac{(\ell-1)!}{\left(\frac{3}{2}\right)_{\ell-1}} \left(\frac{r_<}{r_>}\right)^\ell F\left(\ell,-\tfrac{1}{2};\ \ell+\tfrac{3}{2};\ \frac{r_<^2}{r_>^2}\right) \tag{36a}$$

$$= -\frac{(\ell-1)!}{\left(\frac{3}{2}\right)_{\ell-1}} \frac{r_<^\ell (r_>^2-r_<^2)}{r_>^{\ell+2}} F\left(\ell+2,\tfrac{3}{2};\ \ell+\tfrac{3}{2};\ \frac{r_<^2}{r_>^2}\right) \tag{36b}$$

$$= -\frac{(\ell-1)!}{\left(\frac{3}{2}\right)_{\ell-1}} \left(\frac{r_1 r_2}{r_1^2+r_2^2}\right)^\ell F\left(\tfrac{1}{2}\ell,\tfrac{1}{2}\ell+\tfrac{1}{2};\ \ell+\tfrac{3}{2};\ \frac{4r_1^2 r_2^2}{(r_1^2+r_2^2)^2}\right) \tag{36c}$$

$$= -\frac{(\ell-1)!}{\left(\frac{3}{2}\right)_{\ell-1}} \frac{(r_1 r_2)^\ell}{(r_1+r_2)^{2\ell}} F\left(\ell,\ell+1;2\ell+2;\ \frac{4r_1 r_2}{(r_1+r_2)^2}\right) \quad . \tag{36d}$$

For $\ell = 0$ the differentiation must be applied to the other factors; (19) and (27) yield

$$R_{\log,0} = \log r_> + \sum \frac{(r_< / r_>)^{2s}}{2s(2s-1)(2s+1)} \tag{37a}$$

$$= \log (r_1+r_2) - \tfrac{1}{2} \sum \frac{1}{s(s+1)} \frac{(4r_1 r_2)^s}{(r_1+r_2)^{2s}} \tag{37b}$$

$$= \tfrac{1}{2} \log (r_1^2+r_2^2) - \frac{1}{8} \sum \frac{1}{s(s+\frac{1}{2})} \left(\frac{2r_1 r_2}{r_1^2+r_2^2}\right)^{2s} \tag{37c}$$

the index of summation running from 1 to ∞ in all cases. These series can be summed leading to

$$R_{\log,0} = \log |r_1-r_2| + \frac{(r_1+r_2)^2}{4r_1 r_2} \log \frac{r_1+r_2}{|r_1-r_2|} - \tfrac{1}{2} \quad . \tag{38a}$$

Similarly (36) can be summed for $\ell = 1$, with the result

$$R_{\log,1} = \frac{3}{16} \left(\frac{r_1^2-r_2^2}{r_1 r_2}\right)^2 \log \frac{r_1+r_2}{|r_1-r_2|} - \frac{3(r_1^2+r_2^2)}{8r_1 r_2} \quad . \tag{38b}$$

Differentiation of (30) yields with (35), for $\ell > 0$

$$\frac{r_1^2+r_2^2}{r_1 r_2} R_{\log,\ell} - \frac{2\ell+4}{2\ell+3} R_{\log,\ell+1} - \frac{2\ell-2}{2\ell-1} R_{\log,\ell-1} + \delta_{\ell,1} = 0 \quad , \tag{39}$$

$\delta_{\ell,m}$ being the Kronecker symbol. Similarly (19) can be easily summed for $n = -2$ leading to

$$R_{-2,0} = \log \left\{(r_1+r_2)/|r_1-r_2|\right\} (2r_1 r_2)^{-1} \quad , \tag{40a}$$

$$R_{-2,1} = \frac{3}{4} (r_1^{-2}+r_2^{-2}) \log \left\{(r_1+r_2)/|r_1-r_2|\right\} - \frac{3}{2} (r_1 r_2)^{-1} \quad . \tag{40b}$$

The recurrence relations (30) remain valid for $n = -2$, but in (31)

the limiting ratio $R_{n+2,\ell}(1+\frac{1}{2}n)^{-1}$ is to be interpreted as $2R_{\log,\ell}$ ($\ell > 0$) ; similarly in (32), $R_{n\ell}/n$ tends to $R_{\log,\ell}$ as n tends to zero and $\ell > 0$.

6. Expansion Formulas for Arbitrary Functions of r

The expansion (19) has the advantage that n occurs, as an exponent, for $r_>$ only and, within each gamma product, only in the numerator. This allows the algebraic products to be expressed as products of the operator $(\partial/\partial r_>)$. In fact, we can equate

$$(-\tfrac{1}{2}n)_{\ell+s}(-\tfrac{1}{2}-\tfrac{1}{2}n)_s r_>^{n-\ell-2s} = \frac{(-)^\ell}{2^{2+2s}} r_>\left(\frac{1}{r_>}\frac{\partial}{\partial r_>}\right)^\ell \left[\frac{1}{r_>}\left(\frac{\partial}{\partial r_>}\right)^{2s} r_>^{n+1}\right] \quad (41)$$

so that (19) can be written as

$$R_{n\ell} = (-r_<r_>)^\ell (2\ell+1)\sum_{s=0}^{\infty} \frac{r_<^{2s}}{(2s)!!(2s+2\ell+1)!!} \left(\frac{1}{r_>}\frac{\partial}{\partial r_>}\right)^\ell \left[\frac{1}{r_>}\left(\frac{\partial}{\partial r_>}\right)^{2s} r_>^{n+1}\right] \quad (42)$$

where

$$(2k)!! = 2.4\cdots 2k \quad , \quad 0!! = (-1)!! = 1 \quad ,$$
$$(2k+1)!! = 1.3\cdots(2k+1) \quad . \quad (43)$$

This suggests, for any function $f(r)$ which can be represented as a finite or infinite sum of powers, not necessarily integer,

$$f(r) = \sum c_n r^n \quad , \quad (44)$$

i.e. for essentially all well-behaved functions $f(r)$, that

$$f(r) = \sum_{\ell=0}^{\infty} f_\ell(r_>, r_<) P_\ell(\cos\vartheta_{12}) \quad (45)$$

where

$$f_\ell = (2\ell+1)(-r_<r_>)^\ell \sum_{s=0}^{\infty} \frac{r_<^{2s}}{(2s)!!(2s+2\ell+1)!!} \left(\frac{1}{r_>}\frac{\partial}{\partial r_>}\right)^\ell \left[\frac{1}{r_>}\left(\frac{\partial}{\partial r_>}\right)^{2s} (r_> f(r_>))\right] . \quad (46)$$

This formula can be written symbolically by means of the modified spherical Bessel functions

$$i_\ell(z) = \sum_{s=0}^{\infty} \frac{z^{\ell+2s}}{(2s)!!(2\ell+2s+1)!!} = \left(\frac{\pi}{2z}\right)^{\frac{1}{2}} I_{\ell+\frac{1}{2}}(z) \tag{47}$$

(this is not the notation given in B 7.2.6) as

$$f_\ell = (2\ell+1)(-r_< r_>)^\ell \left(\frac{1}{r_>}\frac{\partial}{\partial r_>}\right)^\ell \left\{\frac{1}{r_>} \frac{i_\ell(r_< \partial/\partial r_>)}{(r_< \partial/\partial r_>)^\ell} \left[r_> f(r_>)\right]\right\} \quad . \tag{48}$$

Similarly (27) can be turned into an operational expansion if we introduce the new variables $\rho = (r_1^2+r_2^2)^{\frac{1}{2}}$ and $r_+ = r_1+r_2$. Thus (27a) leads to

$$f_\ell = \sum_s \frac{(-r_1r_2)^\ell\,(2\ell+1)}{(2s)!!(2s+2\ \ +1)!!} \left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\right)^{\ell+2s} f(\rho) = (2\ell+1)\, i_\ell\left[-\frac{r_1r_2}{\rho}\frac{\partial}{\partial\rho}\right] f(\rho). \tag{49}$$

Similarly (27b) yields

$$\begin{aligned} f_\ell &= \frac{1}{(2\ell-1)!!} \sum \frac{2^s(-r_1r_2)^{\ell+s}(1+\ell)_s}{s!(2+2\ell)_s} \left(\frac{1}{r_+}\frac{\partial}{\partial r_+}\right)^{\ell+s} f(r_+) \\ &= \frac{1}{(2\ell-1)!!} \left(-\frac{r_1r_2}{r_+}\frac{\partial}{\partial r_+}\right)^\ell \Phi\left(1+\ell;2+\ell;\ \frac{-2r_1r_2}{r_+}\frac{\partial}{\partial r_+}\right) f(r_+) \end{aligned} \tag{50}$$

where Φ is the confluent hypergeometric function (B 6). In both (49) and (50) the product r_1r_2 is to be treated as a constant on differentiation. The equivalence of (49) and (50) follows from the connexion of $\Phi(\alpha;2\alpha;2z)$ and the Bessel functions (B 6.9.10)

$$I_\nu(z) = \frac{(\frac{1}{2}z)^\nu}{\Gamma(\nu+1)} e^{-z}\,\Phi(\tfrac{1}{2}+\nu\ ;1+2\nu\ ;2z) \tag{51}$$

which with (47) turns (50) into

$$f_\ell = (2\ell+1)\, i_\ell\left(-\frac{r_1r_2}{r_+}\frac{\partial}{\partial r_+}\right) \exp\left(-\frac{r_1r_2}{r_+}\frac{\partial}{\partial r_+}\right) f(r_+) \quad . \tag{52}$$

Taylor's expansion, which can be written operationally

$$\exp\,(h\,\partial/\partial z)\; f(z) \;=\; f(z+h) \tag{53}$$

and the identity

$$(z^{-1}\partial/\partial z) \;=\; 2\partial/\partial(z^2) \tag{54}$$

shows that (52) is equivalent to

$$f \;=\; (2\ell+1)\; i_{\ell}\left(-\frac{r_1 r_2}{r_+}\frac{\partial}{\partial r_+}\right)\; f\left[(r_+^{\,2}-2r_1 r_2)^{\frac{1}{2}}\right] \tag{55}$$

which is another way of writing (49).

The convergence of the expansions (42), (49) and (50) will not be discussed in detail. Qualitively we can say that for any function $f(r)$ which is analytic for $|r| < M$, the expansions will converge as long as $|r_1|+|r_2| < M$. If $f(r)\cdot r^{-n} (n \neq 0)$ tends to a finite non-zero limit as r tends to zero, this will not affect the convergence for $r_1 \neq r_2$, and even when $r_1 = r_2$, (22) shows that we can expect convergence as long as $n > -2$.

For two types of functions $f(r)$ the expansion (42), (49) and (50) factorize. Let $f(r)$ be a spherically symmetric solution of the wave-equation

$$\nabla^2 f \;=\; r^{-1}\partial^2(rf)/\partial r^2 \;=\; -\,k^2 f \quad , \tag{56}$$

i.e. a spherical Bessel function of order zero of the first, second or third kind (B 7.2.6)

$$\begin{aligned} j_o(r) &= \sin r/r, \quad y_o(r) = -\cos r/r \\ h_o^{(1)}(r) &= -\,ie^{iz}/r, \quad h_o^{(2)}(r) = ie^{-iz}/r \end{aligned} \tag{57}$$

where the same relation as (47) holds between the pairs of functions j_ℓ and $J_{\ell+\frac{1}{2}}$, y_ℓ and $Y_{\ell+\frac{1}{2}}$, and h_ℓ and $H_{\ell+\frac{1}{2}}$. Then in view of (56), the recurrence relations (B 7.11.7-10)

$$w_\ell(z) = (-z)^\ell (z^{-1}d/dz)^\ell w_0(z) \quad , w=j,y,h^{(1)},h^{(2)} \tag{58}$$

and the series expansion for $j_\ell(z)$ which differs from (47) only by the factor $(-)^s$, (45) and (46) lead to

$$w_0(kr) = \sum_\ell (2\ell+1) j_\ell(kr_<) w_\ell(kr_>) P_\ell(\cos\vartheta_{12}) \quad , w=j,y,h^{(1)},h^{(2)} \tag{59}$$

which is Gegenbauer's addition theorem[1] (B 7.15.28,30) particularized to spherical Bessel functions. For the modified Bessel functions i_ℓ and $k_\ell = (\pi/2r)^{\frac{1}{2}} K_{\ell+\frac{1}{2}}$ the corresponding results are in view of (B 7.2.43) and (B 7.11.20)

$$\begin{aligned} i_0(kr) &= \sum (-)^\ell (2\ell+1) i_\ell(kr_<) i_\ell(kr_>) P_\ell(\cos\vartheta_{12}) \\ k_0(kr) &= \sum (2\ell+1) i_\ell(kr_<) k_\ell(kr_>) P_\ell(\cos\vartheta_{12}) \end{aligned} \tag{60}$$

(cf. B 7.6.3); the latter serves as the basis of the zeta function expansion about a common centre in the method by Barnett and Coulson[5] for evaluating molecular integrals.

If $f(r)$ is a Gaussian function

$$f(r) = \exp(-kr^2) \quad , (r^{-1}\partial/\partial r) f(r) = -2kf(r) \tag{61}$$

the expansions (49) and (50) factorize, with the result

$$\exp(-kr^2) = \sum (2\ell+1) i_\ell(2kr_1r_2) \exp\left[-k(r_1^2+r_2^2)\right] P_\ell(\cos\vartheta_{12}) \quad , \tag{62}$$

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[5] M. P. Barnett and C. A. Coulson, Phil. Trans. A <u>243</u>, 221 (1951).

or on dividing by the common exponential

$$\exp(2kr_1r_2\cos\vartheta_{12}) = \sum (2\ell+1)i_\ell(2kr_1r_2)P_\ell(\cos\vartheta_{12}) \quad . \quad (63a)$$

For imaginary values of k this becomes

$$\exp(2ikr_1r_2\cos\vartheta_{12}) = \sum i^\ell(2\ell+1)j_\ell(2kr_1r_2)P_\ell(\cos\vartheta_{12}) \quad ; \quad (63b)$$

these two formulas are equivalent to Sonine's expansion (B 7.10.5) for $\ell = \frac{1}{2}$; (63b) is the well-known expansion for a three-dimensional plane wave in terms of spherical harmonics.

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